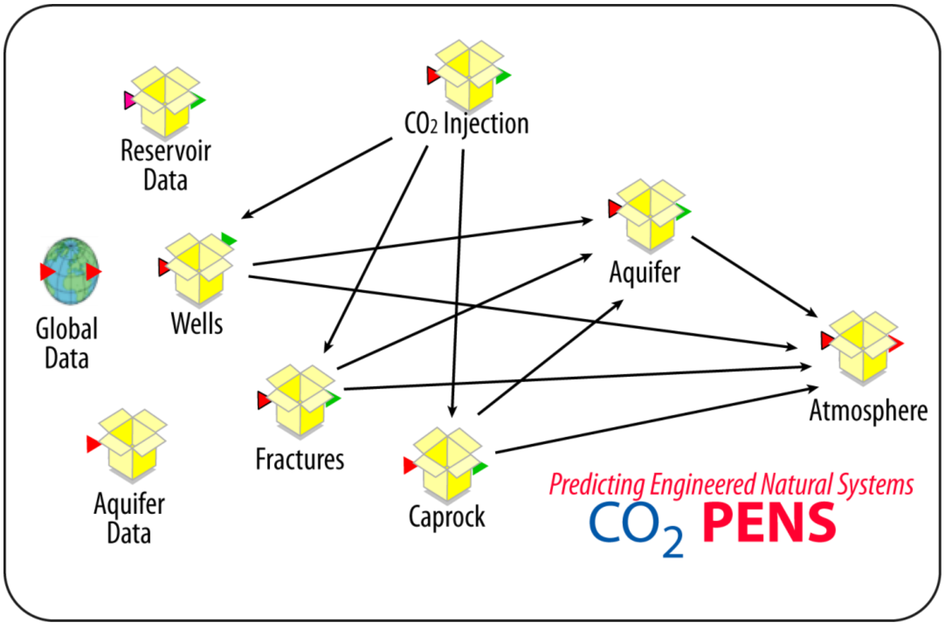

Quantification of Risk Profiles for Atmosphere and Groundwater

25 January 2013

Office of Fossil Energy

NRAP-TRS-III-003-2013

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Cover Illustration: Schematic diagram of the CO_2-PENS system architecture.

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Quantification of Risk Profiles for Atmospheres and Groundwater

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Acronyms and Abbreviations

Term	Description
CCS	CO_2 capture and storage
CO_2-PENS	CO_2-Predicting Engineered Natural Systems
CSLF	Carbon Sequestration Leadership Forum
DLL	Dynamic link library
FEHM	Finite Element Heat and Mass transport code
IAM	Integrated Assessment Model
IPCC	Intergovernmental Panel on Climate Change
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LHS	Latin Hypercube Sampling
LLNL	Lawrence Livermore National Laboratory
LUT	Look-up table
MARS	Multi-variate adaptive regression spline
NRAP	National Risk Assessment Partnership
NETL	National Energy Technology Laboratory
NUFT	Nonisothermal, Unsaturated Flow and Transport with Chemistry code
PNNL	Pacific Northwest National Laboratory
ppm	Parts per million
PSUADE	Problem Solving environment for Uncertainty Analysis and Design Exploration
ROM	Reduced-order model
STOMP	Subsurface Transport Over Multiple Phases
TDS	Total dissolved solids
TOUGH2	Transport Of Unsaturated Groundwater and Heat
UQ	Uncertainty quantification

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1. EXECUTIVE SUMMARY

This report summarizes National Risk Assessment Partnership (NRAP) efforts to develop an approach to quantify risk profiles for atmospheres and aquifers at a CO_2 storage site. We have used a science-based prediction approach for computation of time-dependent profiles for leakage risks at a CO_2 storage site. The approach requires prediction of a storage site performance over long time. We used an Integrated Assessment Model (IAM) in order to implement a system modeling approach for predicting long term site behavior. The systems modeling approach treats a storage site as a system made up of sub-systems such as storage reservoir, overlying seal, wellbores, faults or other transport pathways, and shallow permeable zones including groundwater systems, etc. The behavior of each of the components in the storage-site system is predicted using reduced-order models (ROMs) based on detailed process-level simulations. Different approaches were used to develop ROMs. A look-up table approach, which directly incorporated reservoir simulation results, was used for the storage reservoir; a high-resolution look-up table developed using Lawrence Livermore National Laboratory's (LLNL) PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) package and based on Los Alamos National Laboratory's (LANL) FEHM (Finite Element Heat and Mass transport code) simulation results was used for leakage through cemented wellbores; a look-up table, which directly incorporated simulation results performed using Lawrence Berkeley National Laboratory's (LBNL) TOUGH2 (Transport Of Unsaturated Groundwater and Heat simulator) was used for leakage through open wellbores; high-order polynomial ROMs developed using LLNL's PSUADE package and based on detailed numerical simulations using LANL's FEHM code and Pacific Northwest National Laboratory's (PNNL) STOMP (Subsurface Transport Over Multiple Phases) code were used for shallow aquifers. The IAM was used for first-generation risk profile calculation was built using LANL's CO_2-PENS (CO_2-Predicting Engineered Natural Systems) system model.

A hypothetical storage site consisting of a storage reservoir, wellbores, and a shallow aquifer was used to develop risk profiles for three leakage metrics. The three metrics included volume of a plume of $pH<6.5$ in shallow aquifer, volume of a plume of $TDS > 500$ ppm in shallow aquifer and leakage of CO_2 to atmosphere exceeding a cutoff. We performed Monte-Carlo simulations with 1000 realizations, each sampling from multiple stochastic variables. Results of the Monte-Carlo simulations were used to calculate the risk profiles for the metrics mentioned above as probability of exceeding a given cutoff. The first-generation risk profiles are being used to explore various questions related to long-term performance of a storage site such as what impact does spatial density of wellbores have on whether a site can meet a 99 percent retention criterion. We also performed uncertainty analysis to determine the relative impact of various stochastic variables on the calculated risk profiles.

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2. INTRODUCTION

Deployment of carbon sequestration at large scale requires an efficient, comprehensive scientific approach for assessing both the short- and long-term performance of natural and engineered geologic systems spanning a range of geologic environments. CO_2 storage operations may utilize deep saline formations and will require prediction of CO_2 movement/reactivity over large areas and long periods of time. A range of ongoing field-scale efforts suggest that geologic sites can be exploited to retain large volumes of injected CO_2, although the long-term performance of these systems needs to be assessed confidently with predictive models. To facilitate successful large-scale deployment within the next decade or so, a robust, science-based risk assessment approach is needed for potential uncertainties at specific storage sites to be well enough understood so that data collection and monitoring are optimal and risks minimized.

Ensuring that large-scale CO_2 storage is safe and effective requires predicting the long-term integrity of storage sites as well as demonstrating the comprehensive consideration of potential site-specific risks. The scale of storage sites makes science-based prediction challenging, and the complexity and heterogeneity of natural systems imparts a degree of uncertainty to any predictions, necessitating a stochastic component to the methodology. Most efforts to date have relied on qualitative assessment of risks based on FEPs analysis, which relies on a catalogue of Features of an engineered geologic system that impact its behavior, discrete Events that can impact behavior, and other Processes that can influence its behavior (Cranwell and Guzowski, 1982; Chapman et al., 1995; Nirex, 1998). Quintessa has developed a detailed database of FEPs that has been adapted for geologic storage of CO_2 (Savage et al., 2004; Maul et al., 2005).

A quantitative methodology for predicting a site's long-term performance—going beyond FEPs analysis—is essential to the successful deployment of CO_2 capture and storage (CCS) at a commercial scale, where each storage project will represent significant capital investment and will require sound, quantitative assessments of potential long-term liabilities. Calculation of risk profiles is an approach to assessing the predicted performance of large-scale projects, serving as an important tool for:

- Comparison of potential site options
- Quantification of long-term project costs and potential liabilities
- Providing a basis for both operators and regulators to ensure that sites are characterized and operated in a manner that minimizes key uncertainties and maximizes performance

Quantitative approaches to site performance can range from the process level numerical reservoir simulators to the system level models such as CO_2-PENS (CO_2-Predicting Engineered Natural Systems) (Stauffer et al., 2009). For both types of approaches, accurate quantification of the parameters and process models that describe the engineered geologic system is fundamental to the quality of the simulation and prediction. For geologic systems, the parameters describing a system have uncertainty associated with them. Consequently, uncertainty quantification (UQ) is a critical element of environmental risk assessments. Refsgaard, van der Sluijs, and coworkers (van der Sluijs, 2007; Refsgaard et al., 2006; Refsgaard et al., 2007) present detailed assessments of uncertainties and methodologies for natural systems.

The National Risk Assessment Partnership (NRAP) is developing an approach that relies on the use of integrated assessment models (IAMs) to quantify storage-site performance through calculation of risk profiles. The concept of risk profiles for using risk assessment to quantify potential long-term liabilities was introduced by Benson (2007). Risk profiles provide a time evolution of the probability of a particular risk, thereby allowing an assessment of the risk integrated over a period of time (for example, post closure). Benson noted that potential risks associated with CO_2 storage will be time dependent, largely tracking the evolution of reservoir pressure in response to injection and post-injection recovery and trapping mechanisms. Consequently, Benson predicted that environmental risks will peak with injection and decline as the storage reservoir pressures recover and various near-term and long-term trapping mechanisms come into play. The risk-profile concept has proven very useful in conveying the predicted qualitative evolution of risks. However, the validity of these profiles across a wide range of sites has yet to be confirmed. Quantification of risk profiles is a necessary component in the context of a technical basis for long-term liability. However, no defensible, robust methodology has been developed for quantification of risk profiles for CO_2 storage.

NRAP is utilizing an IAM approach, because it allows treatment of the storage site's geologic complexity, from the reservoir to the potential receptors. With IAMs, the site's behavior is predicted stochastically at the system level using reduced-order models (ROMs). The ROMs are developed using a variety of process-level simulators and/or analytical expressions that represent abstractions (when appropriate) and are based on detailed physical and chemical descriptions of key subsystems at the sites. This approach provides the necessary science-basis to the risk quantification approach. The IAM is used to assess long-term performance of a storage system in order to predict the potential for a specific event or condition to occur, which can then be coupled with a quantification of the event's consequence/impact to derive the risk. .

There is broad international consensus on the main types of risks and adverse impacts that could be associated with the long-term storage of CO_2 (e.g., CSLF, 2009). NRAP is initially focusing on risk profiles associated with several key potential impacts, including:

- Return of CO_2 to the atmosphere
- Groundwater quality
- Reservoir stress that could have adverse impacts on the geosphere

3. INTEGRATED ASSESSMENT MODEL

Development of science-based predictive tools for risk assessment is challenging given the scale and complexity of storage sites. An individual storage site may have a CO_2 plume footprint on the order of 100s of km^2, and the need to consider the behavior of the site's system from the storage reservoir to potential receptors results in a large volume ($>10^3$ km^3) that must be addressed in the predictions that may depend on processes occurring at the nano-scale. Given this scale its challenging to use a single model to predict site-scale behavior based on key processes even at the continuum-scale. Additionally, predicting behavior of multiple heterogeneous natural systems based on a single, site-scale deterministic model is not possible.

Consequently, a standard approach in quantitative environmental risk assessment is to treat the overall site as a group of coupled subsystems, each of which embodies a unique set of physical and chemical characteristics and processes. This approach assumes that these subsystems can be treated without implicit coupling (i.e., they can be treated independently, addressing subsystem coupling explicitly in the integrated assessment model). Such models are analogous to predicting the behavior of an industrial facility by independently predicting the behavior of individual components that are linked via an engineering system model. For quantifying risk profiles, NRAP is exploiting an integrated-assessment-modeling approach based on breaking the storage site into subsystems as illustrated in Figure 1: storage reservoir; potential release mechanisms through wellbores or natural seals; potential receptors (or impact categories).

We are using the CO_2-PENS model (Stauffer et al., 2009), developed with the Goldsim® software package, for building the IAM. GoldSim is a commercially available system modeling package which has been tailored with the unique needs of engineered geologic systems in mind, particularly, uncertainty and heterogeneity. Various approaches can be used to build and implement models for system components using Goldsim. These include analytical expressions, lookup tables, and dynamic link libraries (DLLs) for external executables including process-level models.

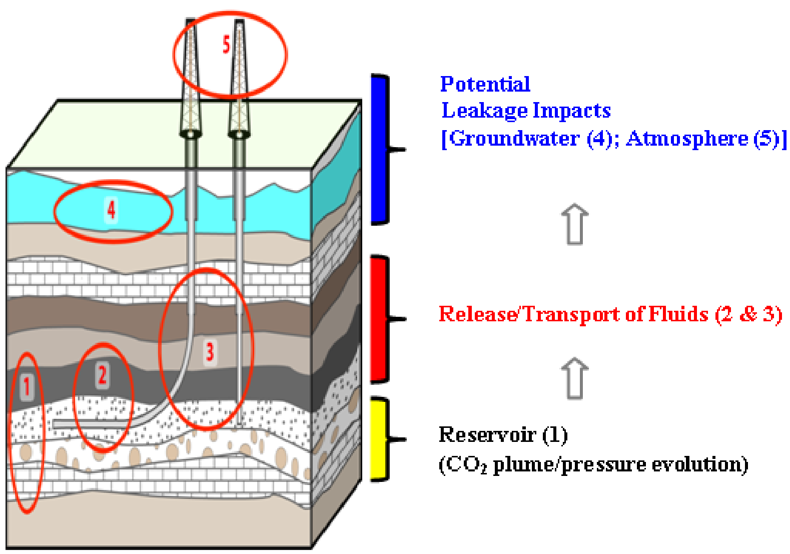

Figure 1: Sub-systems within IAM structure being developed by NRAP.

In order to address uncertainty, the system component models can be executed within a Goldsim model using a Monte Carlo approach, in which parameters are sampled randomly from predefined distributions. Within an IAM, the system components are connected so as to capture the various inter-component interactions at a CO_2 storage site. For example, the component model for the storage reservoir is connected to the component model for a wellbore and the component model for the wellbore is connected to the one for the shallow aquifer, and so on. The inter-component connections are used to capture the mass transfer or pressure transfer between components.

The IAM described here has been developed to assess potential risks due to leakage, including the risk of CO_2 returning to the atmosphere and risks associated with potential impacts to groundwater due to introduction of CO_2 and/or brine. Quantification of these risks requires an IAM that can be used to predict CO_2/brine movement at a storage site over a time period of interest. We used various approaches to build models to describe behavior of storage site sub-system components mentioned above, including, storage reservoir, wellbores and aquifers. Our approach to this IAM is briefly described below.

4. IAM COMPONENT MODELS

The objective of developing the component models is to capture the physical and chemical interactions that will take place as a result of CO_2 injection or migration within the components. In an IAM these models are used to predict how the individual component will behave over a time period of interest. Various approaches can be used to develop component models ranging from abstractions based on detailed process-level simulations to direct incorporation of process simulation results. Our approaches to develop these component models are described below.

4.1 STORAGE RESERVOIR

The reduced order model (ROM) for the storage reservoir is used to predict time-dependent changes in reservoir pressure and saturation (at the reservoir-seal interface) as the result of CO_2 injection. Currently, we are using a look-up table approach in which results of detailed reservoir simulations (from TOUGH2 [Transport Of Unsaturated Groundwater and Heat simulator]) were directly linked as look-up tables. Ultimately, NRAP's goal is to develop a set of options for reduced-order models that allow pressures and saturations to be input from any reservoir simulator; this flexibility will be built into future generations of the NRAP toolset. Our current toolset, however, has a specific reservoir model built in to the CO_2-PENS model.

The reservoir ROM was based on detailed simulations of the Kimberlina reservoir in southern San Joaquin basin in California (Wainwright et al., 2012). It is a saline reservoir that is currently being studied as a potential carbon storage site. The target reservoir is a sandstone formation. A detailed geologic model was developed for the reservoir and was subsequently used to build a numerical simulation model in Lawrence Berkeley National Laboratory's (LBNL) TOUGH2 reservoir simulator. The numerical model was used to perform multiple simulations of large-scale CO_2 injection for 50 years at a rate of 5 million tons/year. Each of the simulation runs was performed for 200 years including 150 years of post-injection relaxation. In all 300 simulation runs were performed to capture the effect of variability in three reservoir parameters including porosity and permeability of target reservoir and permeability of caprock. Sensitivity analysis on these parameters was used to further reduce the 300 runs in 54 representative runs that captured the effect of variability in the reservoir parameters. The time and space-dependent reservoir pressure and saturation results for these 54 runs were brought in the IAM as look-up tables. Each one of the runs was associated with the representative reservoir permeability and porosity and caprock permeability values, such that during the Monte-Carlo calculations a reservoir simulation run can be selected based on a set of the values of uncertain parameters selected for a realization.

4.2 WELLBORES

The ROMs for wellbores are used to calculate the CO_2/brine flow rate through wellbores as a function of the wellbore properties and the pressure and saturation at the reservoir-wellbore boundary. Detailed models were built for two end-member types of wellbores (cemented and open), and these were used to develop the wellbore ROMs.

For cemented wellbores, we used Los Alamos National Laboratory's (LANL) FEHM simulator for the detailed models to predict CO_2 and brine flow up a10-cm diameter wellbore, initially containing pore-space saturated with brine, for 1500 cases over a range of wellbore depth, wellbore cement permeability, and pressure and saturation at the reservoir-wellbore interface.

We assumed that wellbore cement extended over the entire length of wellbore. Input parameter distributions were generated using a Latin Hypercube Sampling (LHS) scheme in Lawrence Livermore National Laboratory's (LLNL) PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration). For the ROM, the results of 1500 FEHM leakage simulation runs were used in PSUADE to generate higher resolution response surfaces for CO_2 and brine leak rate using a MARS (multi-variate adaptive regression spline) fitting scheme. The response surfaces were converted into a multi-dimensional lookup table that was input into the IAM.

For open wellbores, we used the drift-flux model in LBNL's TOUGH2 simulator for the detailed model to predict CO_2 flux through open wellbores. In all, 250 simulation runs were performed by varying wellbore-reservoir boundary pressure, saturation and wellbore depth. The simulated CO_2 and brine leak rates from these runs were converted into a 3-dimensional lookup table for IAM.

It should be noted that both the FEHM and TOUGH2 simulations took into account the complexities of CO_2 phase change during leakage from deeper reservoirs (where CO_2 typically exists in super-critical state) to shallow aquifer or atmosphere (where CO_2 typically exists in gaseous state).

4.3 FAULTS

The ROM for faults/fractures is used to calculate the CO_2/brine flow rate through faults as a function of the fault properties and the pressure and saturation at the reservoir-seal interface.

The model was developed by using results of detailed numerical simulations of CO_2/brine flow along a 2-dimensional fault connecting a storage reservoir and a shallow aquifer. The simulations were performed using LLNL's NUFT (Nonisothermal, Unsaturated Flow and Transport with Chemistry code) simulator. Approximately 900 successful simulation runs were performed by varying pressure and saturation at the intersection of fault with reservoir as well as physical properties of fault (porosity, permeability and thickness), caprock (permeability) and shallow aquifer (permeability & porosity). Similar to the wellbore leakage simulations, the fault simulation models took into account the complexities of phase change during leakage. A sensitivity analysis of the simulation results was used to further reduce the number of variables. Ultimately, the simulation results and the reduced variable set were used in LLNL's PSUADE package to develop ROM for leakage through fault.

The fault ROM was in form of high-order polynomial functions of the primary variables mentioned above.

4.4 CAPROCK

For the first-generation risk-profile toolset, we assumed that the leakage through the caprock was negligible and did not develop a ROM for caprock leakage.

4.5 SHALLOW AQUIFERS

The IAM shallow aquifer model is used to calculate changes in the pH and concentration of total dissolved solids (TDS) in shallow aquifer due to CO_2 and brine leakage. We developed ROMs using LLNL's PSUADE package coupled with results of detailed simulations using process-level models including LANL's FEHM, LLNL's NUFT and Pacific Northwest National Laboratory's (PNNL) STOMP. We developed two reduced-order-models, one for a confined sandstone aquifer and the second for an unconfined carbonate aquifer. For the sandstone aquifer, a numerical simulation model based on the data for High Plains Aquifer in the United States was developed using LLNL's NUFT simulator. For the carbonate aquifers, numerical simulation models based on the data for Edwards' Aquifer in United States were developed using LANL's FEHM and PNNL's STOMP simulators. These numerical models were used to simulate changes in the pH and TDS in the aquifers due to CO_2 and brine leakage in the aquifers.

A set of Monte-Carlo runs were performed by varying values of multiple uncertain parameters, including, aquifer hydraulic properties and geochemical properties. Results of the Monte-Carlo simulations were used to develop ROMs for various quantities of interest using LLNL's PSUADE package. These included dimensions of pH and TDS plumes in shallow aquifer and CO_2 leakage rate out of the aquifer. The ROMs had forms of higher-order polynomial functions of the uncertain parameters. These ROMs were linked using DLLs that can plug in to the IAM developed in Goldsim.

4.6 ATMOSPHERE

For the first-generation risk-profile toolset, we have only focused on CO_2 leak rate to the atmosphere. We did not consider any atmospheric processes post CO_2 leakage that could impact CO_2 concentration in atmosphere directly above the storage reservoir.

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5. CO_2-PENS

5.1 ARCHITECTURE

CO_2-PENS is developed using the GoldSim® system modeling and Monte-Carlo simulation software package. GoldSim has been used extensively in environmental risk assessment applications.[1]

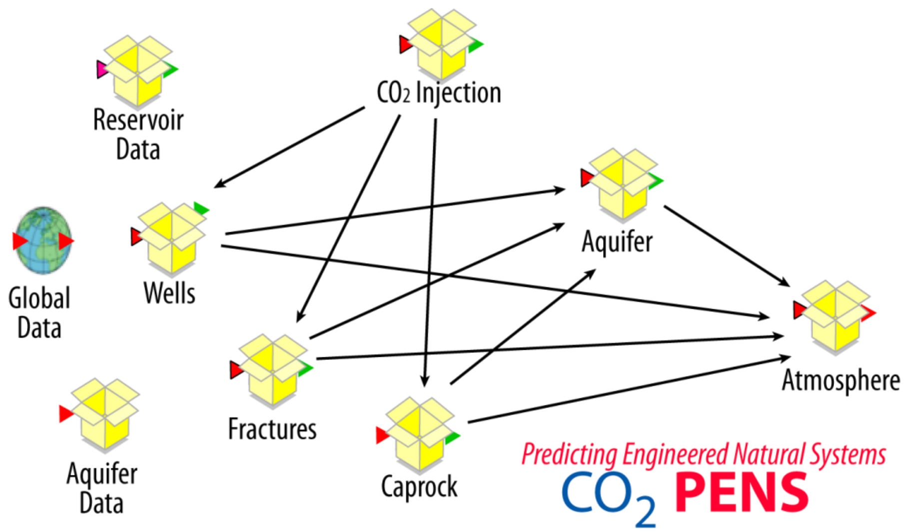

Figure 2: System Model Structure for CO_2-PENS.

The overarching architecture for CO_2-PENS is shown in Figure 2.[2] The model is made up of a number of inter-connected modules (containers) representing various parts of a storage system, including, storage reservoir (CO_2 injection), caprock, faults, wells, shallow aquifer, atmosphere, etc. The connections between the modules capture the connectivities between different storage parts. Each of the modules contain the parameters used to describe the properties of the modules and the ROMs used to calculate the physical/chemical interactions taking place in the module due to CO_2 injection or migration. For example, the injection module represents the storage-reservoir ROM and calculates pressures and saturations at the reservoir–seal interface. It is assumed that wells and faults originate at this horizon. The modules for wells and faults have the ROMs used to calculate CO_2/brine leakage rates between the reservoir and aquifer or atmosphere as a function of pressures and saturations at the reservoir-seal interface and values of parameters such as wellbore cement permeability, fault permeability, etc.

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1 GoldSim is a probabilistic simulation software package that allows simulation of both system dynamics and discrete events; it utilizes a visual and hierarchical modeling environment in which models are constructed models by linking “containers” (e.g., data, equations, etc.) that describe component behavior into a graphical influence diagrams. Influence arrows are used to indicate coupling between containers.

2 The architecture shown here represents the NRAP version of CO_2-PENS. Los Alamos has developed a broader version of CO_2-PENS that includes additional modules for capture, transport, and economics.

As mentioned above, connections between different modules in CO_2-PENS are designed to capture the migration of fluids in a storage system. Figure 3 demonstrates how the reservoir, wellbore and aquifer modules are used to calculate the potential leakage of CO_2 from storage reservoir through the wellbores in a shallow aquifer and the impact of leaked CO_2 in shallow aquifer groundwater quality.

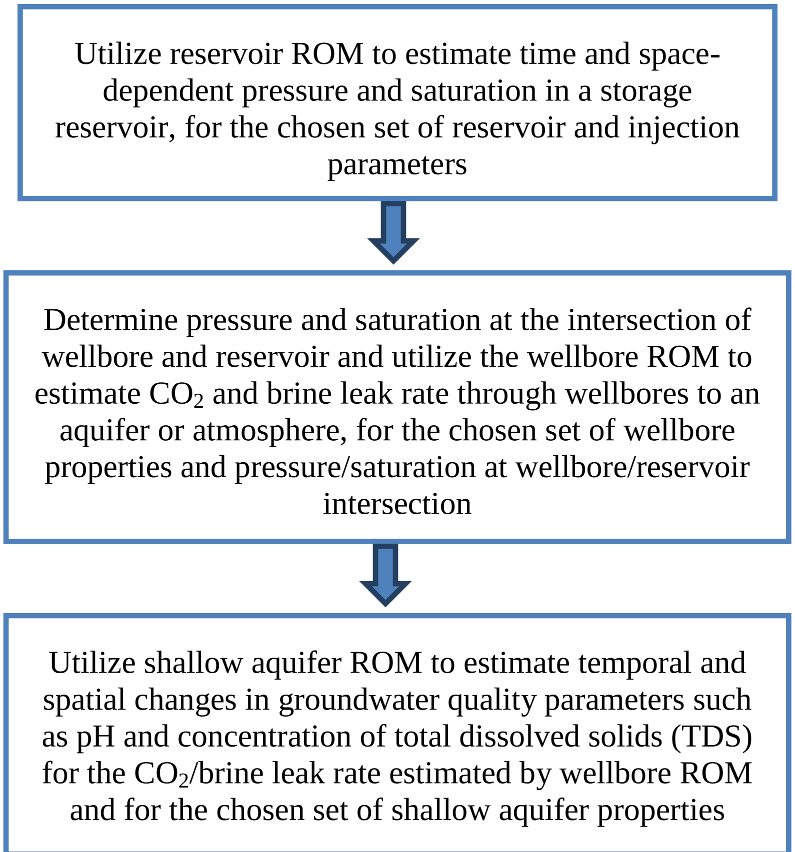


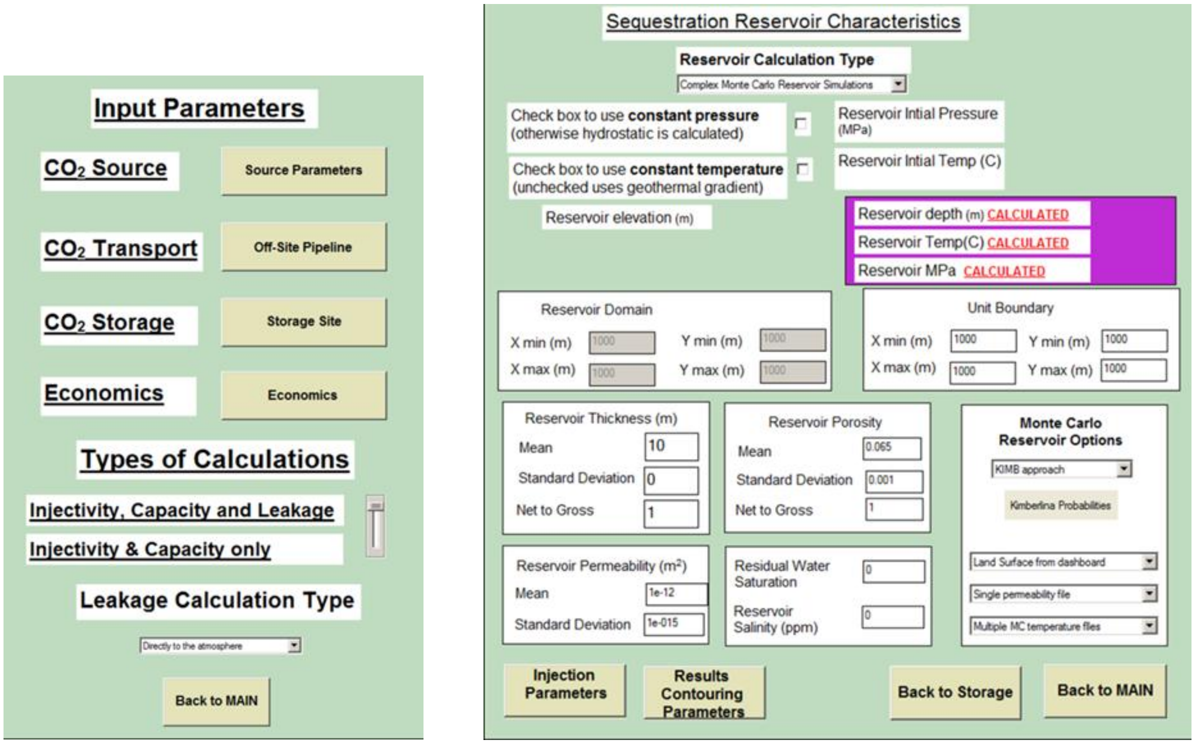
Figure 3: A schematic diagram showing an example of the order of various ROMs used to calculate CO_2 leakage impacts in CO_2-PENS.

5.2 INTERFACE

CO_2-PENS has been set up as a user-friendly model with multiple dashboards that can be used to input parameter values and choose settings for running models. The dashboards include those for CO_2 source, CO_2 transport, and CO_2 storage site. The dashboard for CO_2 storage site can be used to define properties of various parts of a storage site including storage reservoir, wellbores, faults, and shallow aquifers, etc. Figure 4 shows two of the input dashboards. The user can choose to set up the problem using in-built analytical models for two-phase flow in a reservoir or using results of complex reservoir simulations through look-up tables (LUTs) or as ROMs (e.g. a surrogate reservoir model is currently being built based on the Otway field test in Australia and will be used as the ROM). For wellbores and faults, details such as locations, permeability of cements/fault gauge, etc. can be specified. Similarly, details for shallow aquifers such as aquifer depth, thickness, porosity/permeability, etc. can also be specified.

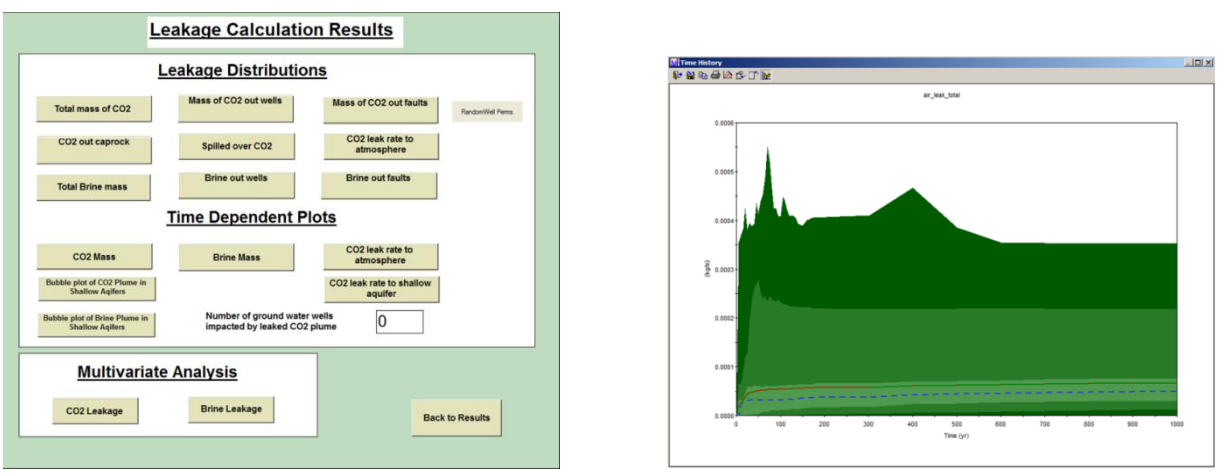
5.3 OUTPUT

Similar to providing inputs, the results of CO_2-PENS calculations are made available through the results dashboard. The results are available either as graphs or tables of computed quantities such as time-dependent leakage rate. Figure 5 shows the main dashboard for accessing various leakage results and an example result.



a) b)

Figure 4: Two of the dashboards used to provide inputs to CO_2-PENS. a) Main input dashboard. b) Dashboard for providing reservoir related inputs.



a) b)

Figure 5: Example for outputs in CO_2-PENS. a) Main output dashboard. b) An example results graph.

Both the graphical and tabular outputs in CO_2-PENS provide statistical measures for Monte-Carlo simulation results, including, mean, standard deviation, confidence intervals, etc. In addition results for all of the individual realizations are available as well. These results can be subsequently used to calculate the probabilities related to failing or exceeding certain performance criteria.

6. EXAMPLE RISK-PROFILE CALCULATION

NRAP's first-generation CO_2-PENS IAM toolset can be used to calculate three leakage related impacts over time, including,

1. Leakage to the atmosphere
2. Change in pH of groundwater
3. Change in concentration of TDS in groundwater

In order to demonstrate one applicability of the first-generation toolset, we provide an example assessment of CO_2 containment in relation to pre-existing wellbores at a site. In this scenario, a key question might be: How does the risk of loss of CO_2 credits vary as a function of wellbores present at site (e.g., wellbore number, wellbore integrity, etc.)?

The risk profiles were calculated using the IAM to perform Monte-Carlo simulations of CO_2 release to the atmosphere. We assumed a hypothetical CO_2 storage site with a target reservoir similar to the Kimberlina reservoir but using a set of leakage pathways that are not applicable to the real site. Specifically, our primary leakage scenario included leakage through hypothetical cemented wellbores that penetrated the storage reservoir, using various numbers, distributions, and permeabilities of the wellbores that represented a range of potential storage site scenarios. Each of the Monte-Carlo realizations simulated performance of a CO_2 storage site over 200 years, which included 50 years of CO_2 injection at 5 million tons/year followed by 150 years post-injection relaxation. Each Monte-Carlo run included 750–1000 realizations, sampling a number of uncertain parameters including:

- Storage reservoir permeability and porosity, caprock permeability
- Wellbore cement permeability, wellbore location, wellbore spatial density

We used multiple different distributions of wellbore cement permeabilities. These distributions were generated based on various sources of data including the sustained casing vent flow and sustained casing pressure data reported for wells in Alberta and Gulf of Mexico, and two permeability distributions based on the low and high wellbore leakage probabilities used in the EIS for FutureGen application. For each of the distributions we performed a separate set of Monte-Carlo runs. The wellbore spatial density was varied between the densities observed at typical oil/gas fields (~ 6–10 wells/km^2) to a density consistent with a saline formation in an area where no prior oil/gas production activity has taken place (1well/100 km^2).

Figure 6 shows example results for calculated CO_2 leak rates for several individual realizations in one of the Monte Carlo simulations. The scenario includes wellbores with cement permeabilities sampled from a distribution derived from ranges reported in an Environmental Impact Statement developed for a potential storage site and wellbore spatial density similar to that of a mature oil/gas field (10 wells/km^2).

The results show that the CO_2 leak rate is dominated by leak characteristics from individual wells, with rate increasing as the reservoir plume intersects a well either during injection or following injection. The net effect is an average probabilistic stochastic leak rate (shown as a red curve on Figure 6) that rises during the injection period and levels off (at least through the 150 years of relaxation that is considered in the simulations). (Although only four realizations are shown on the figure, this red curve reflects the average from 750 realizations.)

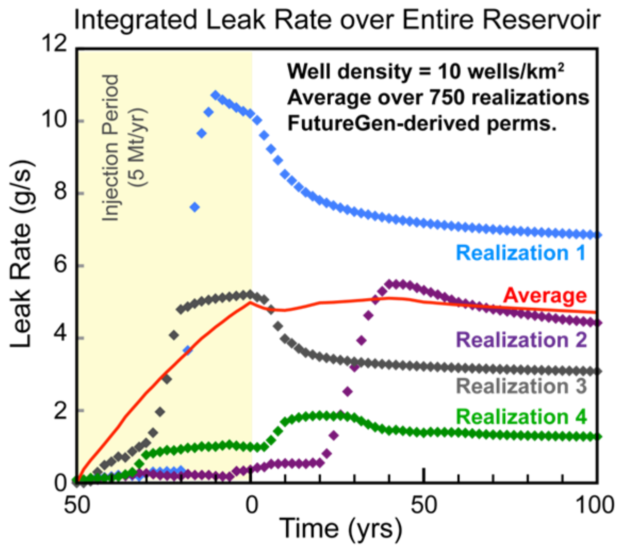


Figure 6: Example leakage rate curves and average leak rate.

The topology of an individual realization for leakage to the atmosphere differs from the topology of the notional risk profile presented by Benson (2007). Specifically, the peak ties more strongly to the timing of when the plume intersects a high permeability wellbore as opposed to tying to the evolution of reservoir pressure. This is to be expected because leakage of CO_2 is driven by CO_2 saturation (plume movement), which evolves at a significantly slower time scale (over multiple decades, depending on reservoir permeability, thickness and depth) compared to pressure front in a saline reservoir (over few years). The evolution of pressure front is inversely proportional to compressibility and since water is very incompressible the pressure effects are felt quicker at farther distance. The net effect is that (1) the leakage peak may occur before or after injection ceases, and (2) the decay of the leakage profile is prolonged relative to the decay of a pressure profile (see Wainwright et al., 2012, Figure 2 a and b for a comparison of the evolution of CO_2 saturation and pressure).

Results of the Monte-Carlo simulations were used to calculate the risk profiles by calculating the probability that the cumulative leak rate exceeds certain cutoffs which will result in failing various CO_2 retention goals such as the IPCC storage goal.

Figure 7 shows an example of the utility of the computed risk profiles. The example demonstrates effect of wellbore spatial density on the percent of CO_2 retained in a storage reservoir over 100 years. The wellbore spatial density was varied between that for typical mature oil/gas fields and very low spatial density. The figure also shows the IPCC storage goal of 99 percent retention for reference. In addition, the figure shows result of the calculation of 1 year of leakage through an open well for reference. (It should be noted that the open well calculation was performed using a different wellbore model that is applicable to the flow conditions in a non-cemented well.) A continuously leaking open well for one year is an unlikely scenario because it could be readily detected and repaired. However, the data point is shown to provide a comparison to an extreme, end-member scenario; further, the calculations are expected to represent a worst-case, in that the reservoir model did not account for trapping mechanisms (which would limit flow over time). Results on Figure 7 demonstrate that for the type of storage system considered in our computation it is possible to meet a 99 percent storage retention goal over the type of time period considered.

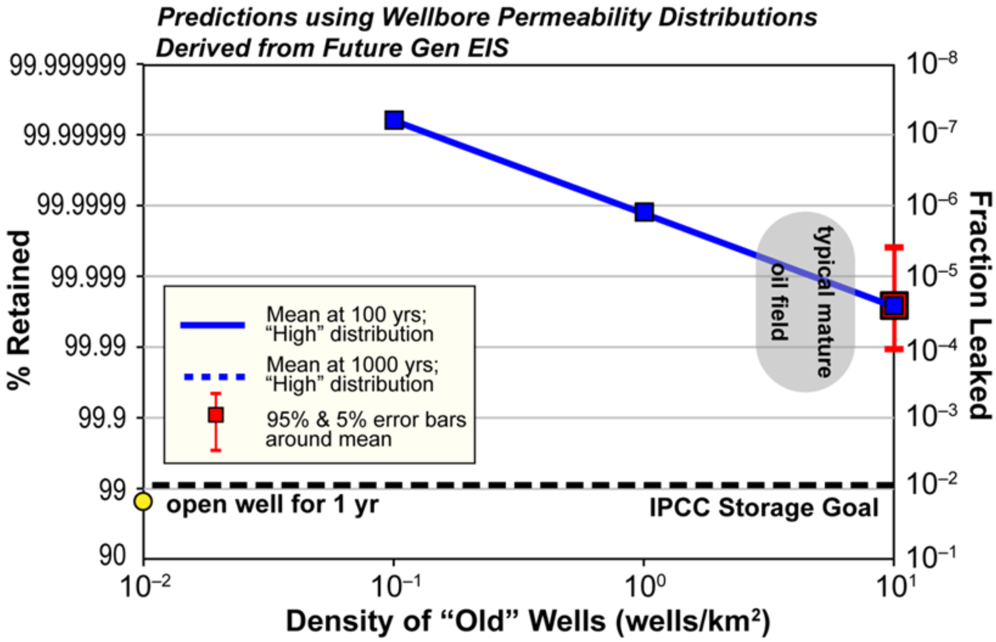


Figure 7: Sub-systems within IAM structure being developed by NRAP.

6.1 UNCERTAINTY QUANTIFICATION CALCULATIONS

The IAM allows an evaluation of uncertainty through the use of Monte Carlo analysis. Our ultimate goal for uncertainty analysis is to identify what uncertain parameters have most influence on the various risks and use the results for developing strategies to minimize uncertainties and mitigate risks. As mentioned above, the uncertain variables in calculations for risks of CO_2 leakage to atmosphere included reservoir parameters (reservoir sand permeability, sand porosity and caprock permeability) and wellbore cement permeability. We used multi-variate analysis to determine how the uncertain variables impact the atmospheric CO_2 leak rate. Table 1 shows the computed correlation coefficients through multi-variate analysis.

Table 1: Correlation coefficients for uncertainty analysis of atmospheric CO_2 leak rate.

Variable	Correlation Coefficient
Wellbore cement permeability	0.869
Caprock permeability	-0.020
Storage reservoir porosity	-0.072
Storage reservoir permeability	-0.104
Wellbore cement permeability	0.869
Caprock permeability	-0.020

As can be seen from Table 1, wellbore cement permeability has a strong influence on the CO_2 leak rate for the sites considered. This is not a surprising result, given that the primary leakage pathway is wellbore and the leak rate through wellbore is strongly influenced by cement permeability. It should also be noted that we assumed that the wellbores are directly connected between storage reservoir and the atmosphere and there are no other intermediate formations where leaked CO_2 can be retained preventing it from going to the atmosphere.

7. CONCLUSIONS

We have developed an IAM to compute risk profiles at a CO_2 storage site. The IAM is built using a system modeling approach and is based on LANL's CO_2-PENS model. The IAM has first-generation ROMs for storage reservoir, wellbores, faults, and shallow aquifer.

We used the IAM to compute risk profiles for impacts due to CO_2 and brine leakage from a storage reservoir through wellbores. The risk profiles have been used to address questions such as effect of wellbore density on CO_2 containment.

The IAM is currently being beta-tested among NRAP partner labs. We intend to share the IAM and associated ROMs with the broader CCS community once the beta-testing is completed.

7.1 IAM LIMITATIONS

We are taking a multi-step approach to developing the ROMs and IAM. We will be developing three generations of ROMs and IAM, where the complexities of the models will increase going from first-generation to third-generation.

- The ROM for storage reservoir was built using results of detailed numerical simulations of CO_2 injection and subsequent flow in a sandstone reservoir. The ROM is limited to a sloping, sandstone reservoir with an open boundary. The CO_2 injection rate is limited to 5 MT/year.
- Two ROMs were built for wellbores, one for open wellbore and second for cemented wellbores. The details of wellbore completions including presence of casing, cement or bridge plugs were ignored. For open wellbore it was assumed that the wellbore is like an open pipe extending from the reservoir to atmosphere or shallow aquifer. For cemented wellbores it was assumed that flow is only through wellbore cement and the cement extends from reservoir to surface. The cement permeability was assumed to be constant with time and the effects of geo-chemical or geo-mechanical interactions due to CO_2 injection or CO_2 migration. We assumed that the residual saturation in cement is zero. Finally, we also assumed that there is no feed-back between wellbore and reservoir due to leakage through wellbore, including, changes in pressure and saturation in the near wellbore region of the reservoir.
- Two ROMs were built for aquifers, one was based on model for a sandstone aquifer and another based on model for a carbonate aquifer. Both the models assumed open aquifer boundaries. The models did not take into account geochemical reactions and were limited to single leakage point (either wellbore or fault). For multiple leak points it was assumed that the principle of superposition can be applied and used it to add results from single leak points.

7.2 PLANS FOR SECOND-GENERATION TOOLSET

As mentioned in previous section, we have developed first generation ROMs and IAM. We are currently in the middle of developing the second-generation ROMs. These ROMs are developed using process-level simulations with increased complexities of underlying processes as described below.

- Reservoir: In addition to the look-up tables based on Kimberlina reservoir simulation runs we will are developing ROMs for two additional types of storage reservoirs. The first one is based on the Otway field test in Australia. We have developed a model for Otway in Schlumberger's Eclipse simulator and are using results of simulations to develop a surrogate reservoir model using a neural network approach. The second type of storage reservoir we are considering is an oil reservoir. We are using an Eclipse simulation model for the SACROC oil reservoir in the Permian basin. While we are using a model for an oil reservoir, our leakage calculations will not have oil as one of the fluids.
- Wellbore: The wellbore ROM for cemented wellbores is being rebuilt for second-generation calculations. We are developing a higher order polynomial function to replace the look-up table used in first-generation. In addition, we are also taking into account the effect of geomechanical processes on cement permeability.
- Aquifer: For second-generation, the aquifer ROMs are being extended to include effect of geochemical reactions as well as leakage through multiple points. In addition to providing the outputs for volumes of pH and TDS plumes, the aquifer ROMs are being developed to provide outputs for volumes of plumes of cadmium, arsenic and lead.

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NRAP is an initiative within DOE's Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide (CO_2). NRAP involves five DOE national laboratories: NETL Regional University Alliance (NETL-RUA), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL). The NETL-RUA is an applied research collaboration that combines NETL's energy research expertise in the Office of Research and Development (ORD) with the broad capabilities of five nationally recognized, regional universities—Carnegie Mellon University (CMU), The Pennsylvania State University (PSU), University of Pittsburgh (Pitt), Virginia Polytechnic Institute and State University (VT), and West Virginia University (WVU)—and the engineering and construction expertise of an industry partner (URS Corporation).

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